Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Understanding and modulating high-energy property of noble-gas hydrides from their long-bonding: an NBO/NRT investigation on $HNgCO^+/CS^+/OSi^+$ and HNgCN/NC (Ng = He, Ar, Kr, Xe, Rn) molecules

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Table S1 CCSD(T) calculated values of the harmonic vibrational frequencies (in cm^{-1}) of HNgAB Molecules

Molecules	H-Ng stretch	Ng-A stretch	A-B stretch	H-Ng-A bend	Ng-A-B bend
$HHeCO^+$	3363.5(3004.6) [a]	318.2(423.4) [a]	2216.1(2285.4) [a]	357.3(439.7) [a]	222.3(203.5) [a]
$HArCO^+$	2737.9(2535.5) [a]	129.0(196.3) [a]	2198.9(2267.4) [a]	272.3(311.7) [a]	140.1(138.7) [a]
$HKrCO^+$	2534.6(2400.5) [a]	124.7(112.7) [a]	2202.7(2268.8) [a]	307.9(314.0) [a]	143.8(130.3) [a]
$HXeCO^+$	2311.4(2213.6) [a]	120.1(172.4) [a]	2202.9(2265.7) [a]	306.4(294.1) [a]	139.0(126.4) [a]
$HRnCO^+$	2185.6	126.7	2207.4	320.3	143.9
$HHeCS^+$	3272.4(3398.9) [b]	411.9(485.2) [b]	1376.9(1336.0) [b]	550.8(556.0) [b]	178.4(190.8) [b]
$HArCS^+$	2691.6(2638.5) [b]	152.0(241.6) [b]	1348.8(1323.4) [b]	392.3(416.0) [b]	123.1(139.6) [b]
$HKrCS^+$	2459.6(2521.1) [b]	141.2(239.8) [b]	1357.7(1325.5) [b]	439.6(432.9) [b]	126.5(139.1) [b]
$HXeCS^+$	2239.7(2278.3) [b]	133.1(230.6) [b]	1359.6(1324.0) [b]	427.9(408.1) [b]	121.0(137.8) [b]
$HRnCS^+$	2108.0	134.9	1365.5	419.5	126.1
$HHeOSi^+$	3549.5(3559.0) [c]	543.2(629.9) [c]	1196.8(1156.0) [c]	462.8(469.0) [c]	146.6(134.7) [c]
$HArOSi^+$	2760.1(2775.6) [c]	199.3(252.3) [c]	1198.0(1162.3) [c]	407.5(412.6) [c]	106.2(105.0) [c]
$HKrOSi^+$	2532.3(2547.2) [c]	178.8(241.4) [c]	1194.6(1158.6) [c]	439.3(442.0) [c]	107.4(105.2) [c]
$HXeOSi^+$	2292.5(2323.2) [c]	166.7(232.6) [c]	1189.3(1155.6) [c]	431.8(428.0) [c]	106.7(106.5) [c]
$HRnOSi^+$	2170.2	166.3	1191.2	412.6	107.6
HHeCN	–	–	–	–	–
HArCN	989.2	309.7	2128.3	664.5	134.5
HKrCN	1597.2	294.0	2138.8	673.0	138.9
HXeCN	1720.7	282.5	2142.7	636.9	139.9
HRnCN	1690.8	280.2	2147.0	573.4	143.7
HHeNC	2428.0	745.7	2050.6	776.7	86.9
HArNC	2217.8	328.1	2050.7	647.3	66.0
HKrNC	2108.7	314.7	2039.3	652.9	80.1
HXeNC	1970.3	306.1	2066.9	615.6	89.7
HRnNC	1886.2	305.7	2070.2	555.1	99.5

[a] From ref. 10. [b] From ref. 11. [c] From ref. 12.

Table S2 Covalent limits R_{cov} and vdW limits R_{vdW} for H−Ng, Ng−A and H−A bonds of HNgAB Molecules

Molecules	$R_{cov,\,H-Ng}$ (Å)	$R_{cov,\,Ng-A}$ (Å)	$R_{cov,\,H-A}$ (Å)	$R_{vdW,\,H-Ng}$ (Å)	$R_{vdW,\,Ng-A}$ (Å)	$R_{vdW,\,H-A}$ (Å)
$HHeCO^+$	0.78	1.21	1.07	2.88	3.24	3.44
$HArCO^+$	1.28	1.71	1.07	3.51	3.87	3.44
$HKrCO^+$	1.49	1.92	1.07	3.66	4.02	3.44
$HXeCO^+$	1.63	2.06	1.07	3.86	4.22	3.44
$HRnCO^+$	1.74	2.17	1.07	3.97	4.33	3.44
$HHeCS^+$	0.78	1.21	1.07	2.88	3.24	3.44
$HArCS^+$	1.28	1.71	1.07	3.51	3.87	3.44
$HKrCS^+$	1.49	1.92	1.07	3.66	4.02	3.44
$HXeCS^+$	1.63	2.06	1.07	3.86	4.22	3.44
$HRnCS^+$	1.74	2.17	1.07	3.97	4.33	3.44
$HHeOSi^+$	0.78	1.09	0.95	2.88	3.05	3.25
$HArOSi^+$	1.28	1.59	0.95	3.51	3.68	3.25
$HKrOSi^+$	1.49	1.80	0.95	3.66	3.83	3.25
$HXeOSi^+$	1.63	1.94	0.95	3.86	4.03	3.25
$HRnOSi^+$	1.74	2.05	0.95	3.97	4.14	3.25
HHeCN	–	–	–	–	–	–
HArCN	1.28	1.71	1.07	3.51	3.87	3.44
HKrCN	1.49	1.92	1.07	3.66	4.02	3.44
HXeCN	1.63	2.06	1.07	3.86	4.22	3.44
HRnCN	1.74	2.17	1.07	3.97	4.33	3.44
HHeNC	0.78	1.17	1.03	2.88	3.13	3.33
HArNC	1.28	1.67	1.03	3.51	3.76	3.33
HKrNC	1.49	1.88	1.03	3.66	3.91	3.33
HXeNC	1.63	2.02	1.03	3.86	4.11	3.33
HRnNC	1.74	2.13	1.03	3.97	4.22	3.33

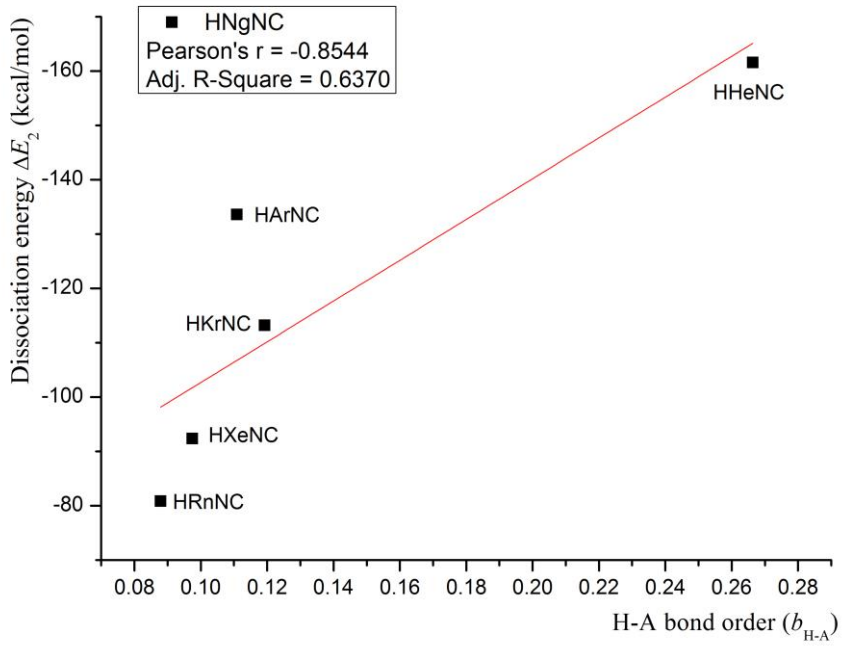

Figure S1. Correlation plot for long-bond orders ($b_{H–A}$) – dissociation energies (ΔE_2) of HNgNC species.

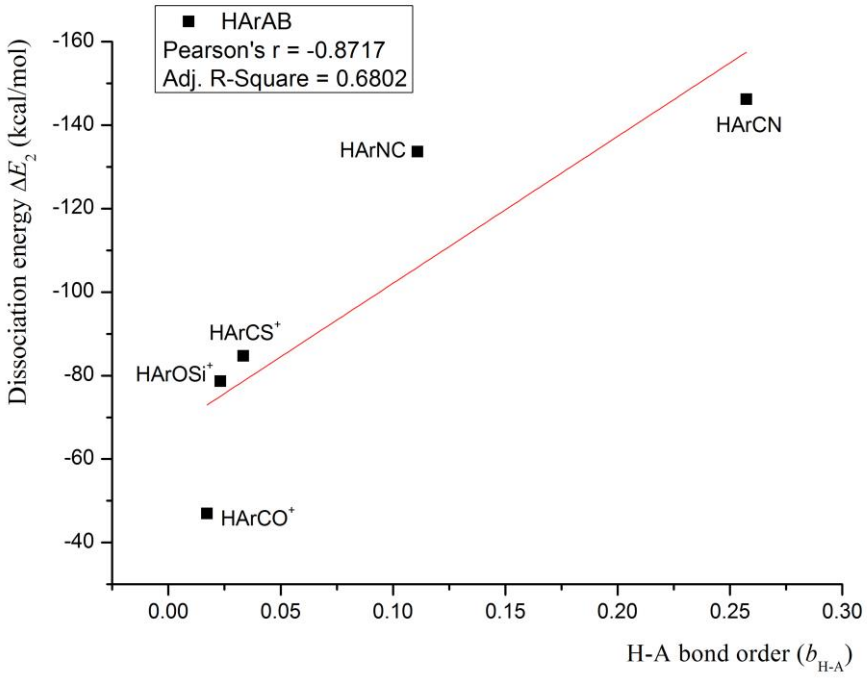

Figure S2. Correlation plot for long-bond orders ($b_{H–A}$) – dissociation energies (ΔE_2) of HArAB species.

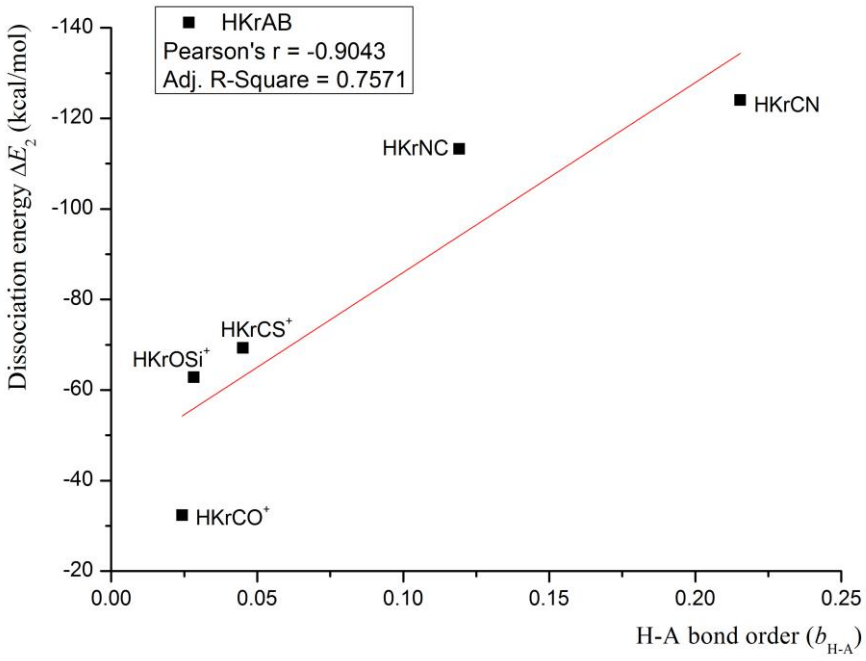

Figure S3. Correlation plot for long-bond orders ($b_{H–A}$) – dissociation energies (ΔE_2) of HKrAB species.

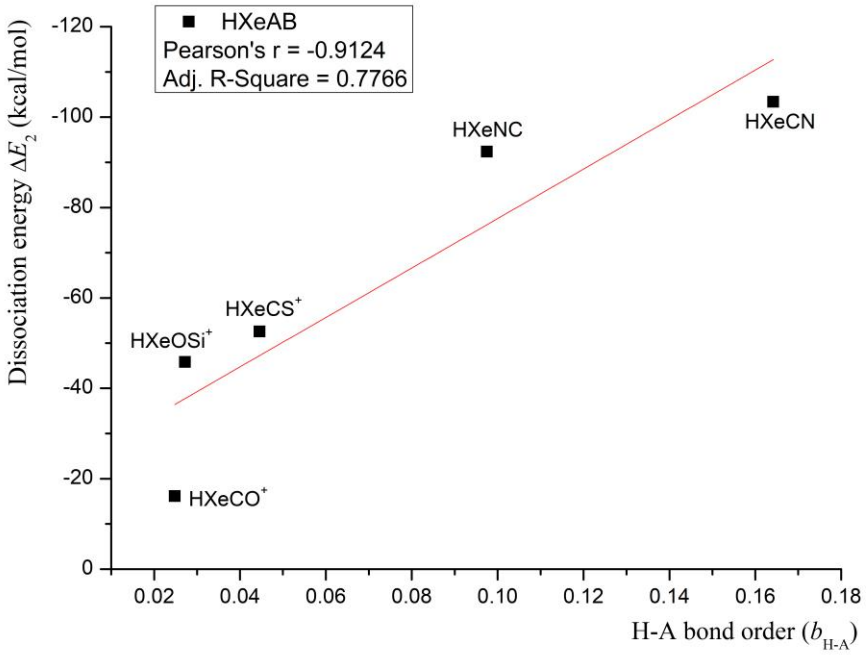

Figure S4. Correlation plot for long-bond orders ($b_{H–A}$) – dissociation energies (ΔE_2) of HXeAB species.

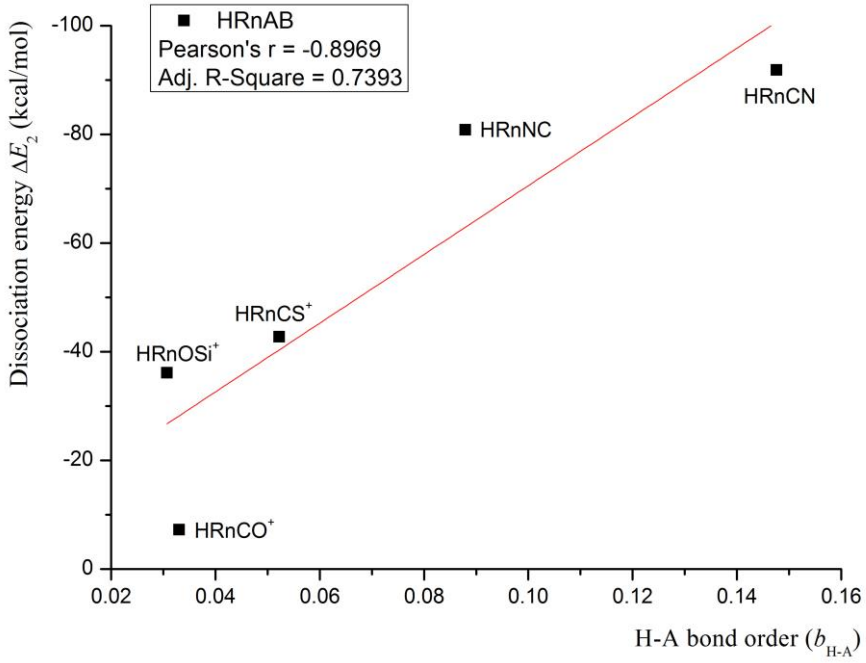

Figure S5. Correlation plot for long-bond orders ($b_{H–A}$) – dissociation energies (ΔE_2) of HRnAB species.